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The Physical Mechanism of Proton Transfer in Proteins

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Proteins are able to perform an enormous variety of functions, while using only a limited number of underlying processes. One of these is proton transfer. The physical mechanism of proton transfer has been extensively studied, using a variety of experimental and computational methods. However, it remains unclear what determines the direction and rate of proton transfer reactions in proteins. We have developed and applied a new approach to this long-standing problem by integrating structural dissection, energy landscape, first principle calculation (quantum theory), and molecular dynamics simulation. Our proof of concept study reveals key structural elements that control the direction and rate of proton transfer in proteins. The results are of predictive power and can be generally applied to different proteins.